

Petascale Plasma Physics Simulations on Roadrunner Using VPIC

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For many problems of interest in kinetic plasma physics, including laser plasma interactions and magnetic reconnection, the particle-in-cell (PIC) method is the only viable simulation tool. Members of the VPIC team are using this method to pioneer discoveries in areas such as inertial confinement fusion (ICF) research at the National Ignition Facility (NIF).

VPIC [1], a highly optimized, state-of-the-art PIC implementation for fully relativistic, 3D, explicit, kinetic plasma simulations, has been specifically designed to minimize data motion, an increasingly important computational consideration, as modern processing architectures consume more time in moving data than in performing computations. Additionally, VPIC aggressively makes use of the short-vector, single instruction multiple data (SIMD) execution pipelines available on many of these architectures.

Recent work by X-1-PTA and CCS-2 staff has resulted in the adaptation of VPIC to run efficiently on the IBM Cell Broadband Engine (Cell BE) chip, which forms the basis of the new petaflop/s Roadrunner supercomputer that LANL will acquire in 2008. The VPIC particle-push performance on this hardware is staggering, at 0.17 billion cold particle advances per second per Cell BE. This opens the possibility of simulating plasmas on the full Roadrunner system as large as one trillion particles, one billion computational cells, and one million time integrations in 10 days of wall-clock time, a simulation scale 10 times larger than what is feasible today.

VPIC has been applied with success in both basic and applied science. In Fig. 1, we show electron density isosurfaces resulting from magnetic reconnection of a Harris geometry (a plasma equilibrium with a reversal of magnetic field across a neutral layer, with pressure equilibrium established by an initial region of high density at the sheet center) in the case of an intermediate guide field. The simulation follows the dynamics of 16 billion particles on a $1000 \times 100 \times 1000$ mesh (physical domain $200 \times 20 \times 200 d_i$, where d_i is the ion inertial length). The color indicates magnetic field strength B_y (y is the direction of the initial current) at a time when the

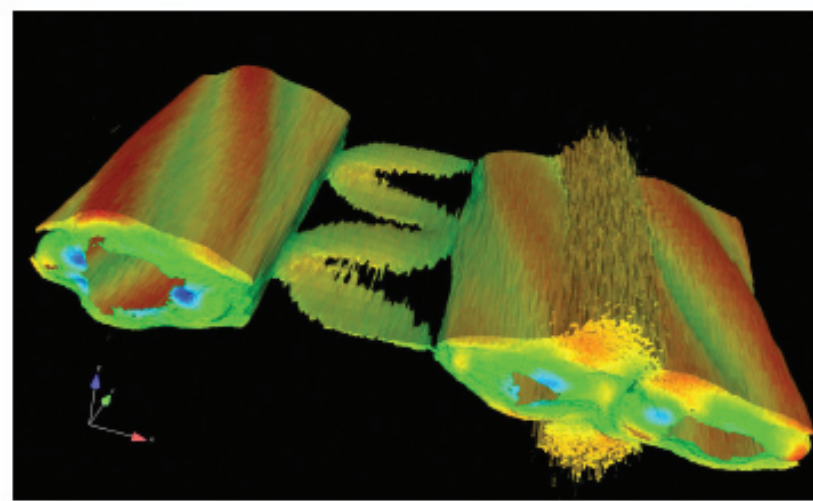


Fig. 1. VPIC simulations of magnetic reconnection in a pair plasma with an intermediate guide field. Displayed are isosurfaces of electron density colored by the magnetic field B_y (y is in the initial current and guide field direction). The isosurfaces undulate from interaction of the tearing modes (wave vector along x) with the drift-kink modes (along y).

dominant diffusion region has formed and is influenced by a current-aligned instability, the drift-kink mode [2]. This calculation required 36 hours of wall-clock time on 500 AMD Opteron cores.

In Fig. 2, we show a 3D simulation of stimulated Raman scattering (SRS) in the kinetic regime ($kl_d = 0.34$, where k is the initial Langmuir wavenumber and l_d is the plasma Debye length). The simulation used 18 billion particles on a mesh of size $2436 \times 486 \times 486$ (a physical domain $90 \times 18 \times 18$ microns) run on 1008 AMD Opteron cores. The electron plasma waves self-localize to regions of narrow transverse extent, as shown by the filament structures in the longitudinal electric field. SRS saturates via the trapped electron self-focusing of Langmuir waves [3]. SRS is one of the pernicious instabilities that jeopardize the success of realizing inertial confinement fusion ignition at the multi-billion-dollar NIF at Lawrence Livermore National Laboratory.

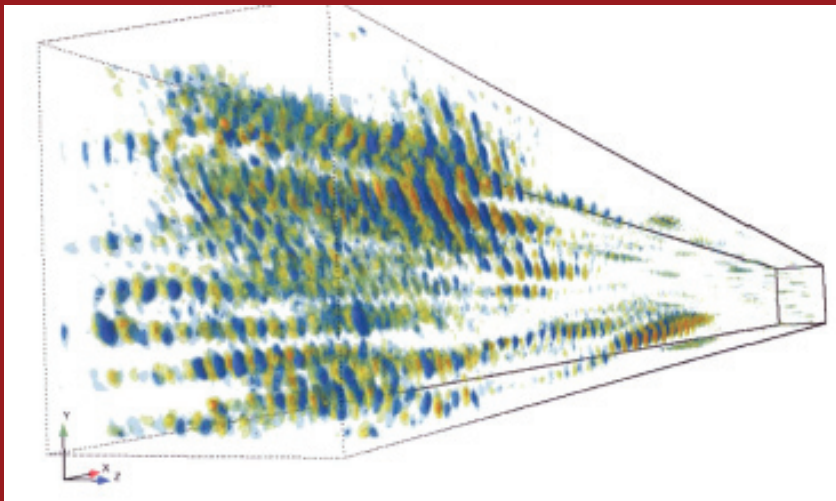


Fig. 2. VPIC simulations of stimulated Raman scattering (SRS) in the kinetic regime. Isosurfaces of longitudinal electrostatic field show filament structures resulting from trapped electron self-focusing of Langmuir waves during SRS saturation. The laser is launched from the simulation geometry near face.

The combined abilities of VPIC to provide excellent science with exceptional computational efficiency make it a natural candidate for adaptation to the Roadrunner hybrid supercomputing architecture. With the development of a working hybrid code, the VPIC team has already made outstanding progress towards ensuring that petascale plasma physics simulations on this exciting new resource become a reality.

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- [1] K. J. Bowers, et al., "Ultra high performance 3D electromagnetic relativistic kinetic plasma simulation," *Phys. Plasmas* (in press).
- [2] L. Yin et al., "Fully kinetic 3D simulations of collisionless reconnection in large-scale plasmas," *Phys. Rev. Lett.* (submitted).
- [3] L. Yin et al., *Phys. Rev. Lett.* **99**, 265004 (2007).

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